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## Numerical Methods for Systems with Measurable Coefficients

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We give a new family of numerical algorithms to solve the initial value problem for the  $n$ -dimensional system

$$dy/dt = f(t, y), \quad y(t_0) = y_0$$

in which  $f$  is smooth in space ( $y$ ) but only bounded and measurable in  $t$  ( $t$ ). Understanding “solution” in the sense of an absolutely continuous solution of

$$y(t) = y_0 + \int_{t_0}^t f(s, y(s)) ds,$$

this problem falls easily within the scope of standard local existence and uniqueness arguments by Picard iteration. What seems less evident is that this formulation can often provide a useful model for quite ordinary problems which at first sight do not appear to require such mathematical generality. This can be illustrated by problems in which  $f$  undergoes rapid time variations of moderate size which for economic or other practical reasons cannot be followed in detail. For example, it might even be that  $f$  is analytic in  $t$  but varies so rapidly that in a slow time scale (perhaps the only scale available to us, say, in the press of real time computation) even its continuity cannot be discerned. One source of such problems is the analysis of systems of the form

$$dy/dt = \lambda Ay + g(t, y)$$

where  $\lambda$  is large,  $A$  is Hamiltonian, and  $g$  is moderate in size. The change of variable  $y = \exp\{\lambda At\}z$  leads to the equivalent system

$$dz/dt = \exp\{-\lambda At\}g(t, \exp\{\lambda At\}z)$$

in which the large linear term has been removed at the cost of replacing the moderately sized, moderately varying perturbation  $g$  by a rapidly varying one. However, such examples only represent an extreme part of the useful range of this model. What is this range? We will argue that it consists of *problems in which  $f$  varies significantly faster in time than in space.*

We propose a family of numerical methods for such systems. It is loosely akin to the Runge-Kutta family in its construction from self-substitutions of  $f$ . However, our hypothesis that  $f$  is only measurable in  $t$  suggests the premise (at least in principle) that the value of  $f(\cdot, y)$  at a single point does not contain much reliable information. We therefore first discretize with respect to  $y$  alone, retaining dependence on  $t$  only through mean properties. Specifically we allow mean values of  $m$ -fold self-substitutions of  $f$  depending on  $f$  at  $m$  different values of  $t$ . Of course such partial discretization does not yield a numerical method. But by estimating the resulting means with Monte Carlo simulation we then obtain actual

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numerical procedures which simulate estimators in the statistical sense for the solution. It is well appreciated (and obvious) that this step is intrinsically parallelizable with slight overhead. This is crucial for our methods, and it is primarily *comparisons on the basis of total computation time assuming high parallelism*, that show our algorithms to significant advantage. We call these Runge-Kutta Monte Carlo or RKMC methods. We adopt the convention that the "order" of a method is the order in a characteristic step size assuming that the stochastic error introduced by Monte Carlo simulation is not dominant (even though it may dominate in actual calculation with a certain probability [3]). To obtain higher order methods we require a preliminary, benchmark family of methods generated by functional Taylor expansion of  $y(t)$  in its dependence on  $f$ . Since our methods are single-step it will suffice to specify a numerical approximation  $Y_1$  for  $y(t_0 + h)$  in terms of  $Y_0 = y(t_0)$ . These formulas are more complicated than their Runge-Kutta counterparts precisely because our weak hypotheses preclude any advantageous combination of values of  $f$  at different values of  $t$ . We give our formulas in scalar form, but remark that, in the proper language of vector-multilinear calculus, all remain literally true for higher dimensional systems. We use  $E_m$  to denote expectation over the uniform distribution on the  $m$ -cell  $[t_0, t_0 + h]^m$ , a subscript  $y$  to denote spatial differentiation, and a hat (  $\hat{\phantom{x}}$  ) above a component of a vector to indicate that it has been deleted.

**THEOREM.** Assume that the initial value problem

$$dy/dt = f(t, y), \quad y(t_0) = y_0$$

has a solution  $y(t)$  on the interval  $[t_0, t_0 + h]$  and that  $f$  is smooth in  $y$  and bounded and measurable in  $t$ . Let the random variables  $U_1, \dots, U_m$  be the nonincreasing rearrangement of  $m$  independent random variables uniformly distributed on  $[t_0, t_0 + h]$ . Then for each  $m$ ,  $y_1 = y(t_0 + h)$  satisfies a relation of the form

$$y_1 = y_0 + hE_m\{F_m(U_1, \dots, U_m; y_0)/m!\} + O(h^{m+1})$$

where the  $F_m$  are given by the recursion scheme

$$\begin{aligned} H_0(y) &= y, \quad F_0 = 0, \\ H_{m+1}(t_1, \dots, t_{m+1}; y) &= H_{m\mathbf{y}}(t_1, \dots, t_m; y)f(t_{m+1}; y), \\ F_{m+1}(u_1, \dots, u_{m+1}, y) &= \sum_{1 \leq j \leq m+1} F_m(u_1, \dots, \hat{u}_j, \dots, u_{m+1}; y) \\ &\quad + h^m H_{m+1}(u_1, \dots, u_{m+1}; y). \end{aligned}$$

To indicate the proof, let the asymptotic expansion of  $y(t)$  as a functional power series in  $f$  be

$$y(t) \sim y(s) + \int_s^t H_1\{t_1; y(s)\} dt_1 + \int_s^t \int_s^{t_1} H_2\{t_1, t_2; y(s)\} dt_2 dt_1 + \dots$$

where  $H_m = H_m\{t_1, \dots, t_m; y\}$  is a homogeneous functional of degree  $m$  depending on values of  $f$  and its derivatives at  $t_1, \dots, t_m$ . Applying  $d/ds|_{y(s)=y_0}$  we obtain

$$0 = f(s, y_0) - H_1\{s; y_0\} + \int_s^t H_{1\mathbf{y}}\{t_1; y_0\} f(s, y_0) dt_1 - \int_s^t H_2\{t_1, s; y_0\} dt_1 + \dots$$

Equating homogeneous terms of each degree yields the recursion scheme for the  $H_m$ . Various manipulations exploiting symmetry then unite all integrals up to a given order into a single integral over a common cell. Reinterpreting this integral as an expectation completes the proof.

Carrying out the recursion we obtain explicit formulas. For efficiency in notation in the following corollary we use a subscript  $k$  to denote evaluation at  $t = U_k$ , and suppress explicit reference to the argument  $y_0$  which appears uniformly as the second argument in all function values.

COROLLARY. Under the same hypotheses, the following single-step approximations to  $y_1 = y(t+h)$  are correct to the indicated order.

- A.  $y_1 = y_0 + hE_1\{f_1\} + O(h^2)$ .
- B.  $y_1 = y_0 + (h/2)E_2\{f_1 + f_2 + hf_{y_1f_2}\} + O(h^3)$ .
- C.  $y_1 = y_0 + (h/6)E_3\{2f_1 + 2f_2 + 2f_3 + hf_{y_1f_2} + hf_{y_1f_3} + hf_{y_2f_3} + h^2f_{y_1f_2f_3} + h^2f_{y_2f_1f_3}\} + O(h^4)$ .

D.

$$\begin{aligned} y_1 = Y_0 + (h/24)E_4\{ & 6f_1 + 6f_2 + 6f_3 + 6f_4 \\ & + 2h(f_{y_1f_2} + f_{y_1f_3} + f_{y_1f_4} + f_{y_2f_3} + f_{y_2f_4} + f_{y_3f_4}) \\ & + h^2(f_{y_1f_2f_3} + f_{y_1f_2f_4} + f_{y_1f_3f_4} + f_{y_2f_3f_4} \\ & + f_{y_2f_1f_3} + f_{y_2f_1f_4} + f_{y_2f_3f_4} + f_{y_3f_2f_4}) \\ & + h^3(f_{y_1f_2f_3f_4} + 2f_{y_2f_1f_3f_4} + f_{y_2f_1f_2f_4} \\ & + f_{y_1f_2f_3f_4} + f_{y_2f_1f_2f_3f_4})\} + O(h^5). \end{aligned}$$

To describe actual algorithms, we introduce an operator representing Monte Carlo simulation of the special expectations in these formulas. Here it is convenient to indicate the domain of  $F$  explicitly by dummy (lower case) variables.

DEFINITION. Let  $\{T_{ij}\}$  be an  $m$  by  $p$  array of independent random variables uniformly distributed on the interval  $[t_0, t_0 + h]$ . For each fixed  $i$ , let  $U_{ij}$  be the nonincreasing rearrangement of  $T_{ij}$ . Given  $F: R^m \rightarrow R^n$ , define the operator  $E_{mp}$  by

$$E_{mp}\{f(u_1, \dots, u_m)\} = \frac{1}{p} \sum_{1 \leq j \leq p} F(U_{1j}, \dots, U_{mj}).$$

In terms of this operator and the polynomial functionals  $F_m$  of the preceding theorem we can define a counterpart of the Taylor family of algorithms. The  $p$ -fold parallel Taylor Monte Carlo or TMC method of order  $m$  consists of successive independent steps of the form

$$Y_1 = Y_0 + hE_{mp}\{F_m(u_1, \dots, u_m; Y_0)\}.$$

Finally we obtain explicit RKMC formulas by assembling self-substitutions into constellations having Taylor expansions in  $h$  agreeing to a given order with a TMC method. The search for higher order formulas, as with proper Runge-Kutta methods [1], [2], especially those enjoying valuable subsidiary properties, leads to substantial algebraic complexities. The general pattern is a linear combination of explicit successive substitutions in which nested function evaluations at the ordered random times  $U_1, U_2 \dots U_m$  are time ordered in the sense that function evaluations deeper in a single successive substitution cannot occur later. Thus, for example,  $f(U_1, y_0 + hf(U_2, y_0))$  can appear but not  $f(U_2, y_0 + hf(U_1, y_0))$ .

DEFINITION. An explicit  $p$ -fold parallel RKMC method is given by formulas of the form

$$\begin{aligned} Y_1 &= Y_0 + hE_{mp}\{\sum_r \sum_i b_{ir} k_i^{(r)}(u_{m-r+1}, \dots, u_m)\}, \\ k_i^{(r)} &= hf(u_r, Y_0 + \sum_r \sum_i a_{ij}^{rs} k_j^{(s)}(u_{m-s+1}, \dots, u_m)), \end{aligned}$$

where  $1 \leq r \leq m$ ,  $1 \leq j \leq M$ , and

$$a_{ij}^{rs} = 0 \text{ if } r \geq s.$$

We note that the strict time ordering ensures that the method is explicit.

The simplest example and essential prototype of the RKMC family is

$$1. Y_1 = Y_0 + hE_{1p}\{f(u_1, Y_0)\}.$$

We have carried out a detailed error analysis of this method by combining deterministic perturbation techniques with martingale estimates [3]. However, for actual calculation, higher order methods are more interesting. In close analogy with a family of second order Runge-Kutta methods there is a one parameter family of second order RKMC methods. Given the real parameter  $\alpha$ ,  $y_1 = y(t_0 + h)$  satisfies

$$y_1 = y_0 + \frac{h}{2} E_2 \left\{ \frac{1}{\alpha} f(U_1, y_0 + \alpha h f(U_2, y_0)) \right. \\ \left. + \left(1 - \frac{1}{\alpha}\right) f(U_1, y_0) + f(U_2, y_0) \right\} + O(h^3).$$

As special cases, for  $\alpha = 1$  and  $\alpha = 1/2$  we obtain methods loosely akin to the trapezoidal and midpoint quadrature methods. However their specific form seems less than obvious.

$$2. Y_1 = Y_0 + \frac{h}{2} E_{2p} \{ f(u_1, Y_0 + h f(u_2, Y_0)) + f(u_2, Y_0) \}.$$

$$3. Y_1 = Y_0 + h E_{2p} \left\{ f(u_1, Y_0 + \frac{h}{2} f(u_2, Y_0)) + \frac{1}{2} f(u_2, Y_0) - \frac{1}{2} f(u_1, Y_0) \right\}.$$

A family of third order algorithms is generated by

$$y_1 = y_0 + \frac{h}{6} E_3 \left\{ \frac{1}{\alpha} f(U_1, y_0 + \frac{\alpha h}{1-\lambda} f(U_2, y_0 + (1-\lambda) h f(U_3, y_0))) + \frac{\alpha h}{1-\mu} f(U_3, y_0) \right. \\ \left. - \frac{\lambda^2}{\alpha} f(U_1, y_0 + \frac{\alpha h}{\lambda(1-\lambda)} f(U_2, y_0)) - \frac{\mu^2}{\alpha} f(U_1, y_0 + \frac{\alpha h}{\mu(1-\mu)} f(U_3, y_0)) \right. \\ \left. + \left(2 - \frac{1}{\alpha} [1 - \lambda^2 - \mu^2]\right) f(U_1, y_0) \right. \\ \left. + \frac{1}{\beta} f(U_2, y_0 + \frac{\beta}{1-\rho} h f(U_3, y_0)) - \frac{\rho^2}{\beta} f(U_2, y_0 + \frac{\beta}{\rho(1-\rho)} h f(U_3, y_0)) \right. \\ \left. + \left(2 - \frac{1}{\beta} [1 - \rho^2]\right) f(U_2, y_0) + 2 f(U_3, y_0) \right\} + O(h^4)$$

where  $\alpha = (1-\lambda)(1-\mu)$ .

The choice  $\lambda = \mu = \rho = 1/2$ ,  $\alpha = \beta = 1/4$  gives a concrete example of a third order formula:

$$4. Y_1 = Y_0 + \frac{h}{6} E_{3p} \left\{ 4 f(u_1, y_0 + \frac{h}{2} f(u_2, Y_0 + \frac{h}{2} f(u_3, Y_0))) + \frac{h}{2} f(u_3, Y_0) \right. \\ \left. - f(u_1, Y_0 + h f(u_2, Y_0)) - f(u_1, Y_0 + h f(u_3, Y_0)) \right. \\ \left. + 4 f(u_2, Y_0 + \frac{h}{2} f(u_3, Y_0)) - f(u_2, Y_0 + h f(u_3, Y_0)) \right. \\ \left. - f(u_2, Y_0) + 2 f(u_3, Y_0) \right\}.$$

If  $f(t, y)$  is independent of  $t$  then this agrees with the (unfamiliar) Runge-Kutta scheme

$$k_1 = h f(t_0, Y_0) \\ k_2 = h f(t_0, Y_0 + k_1) \\ k_3 = h f(t_0 + \frac{h}{2}, Y_0 + \frac{1}{2} k_1) \\ k_4 = h f(t_0 + h, Y_0 + \frac{1}{2} k_3 + \frac{1}{2} k_1) \\ Y_1 = Y_0 + \frac{2}{3} k_4 + \frac{2}{3} k_3 - \frac{1}{2} k_2 + \frac{1}{6} k_1.$$

This algorithm requires four function evaluations to yield a third order method. However, emphasizing again that we take for granted parallel computation of function values, the salient number is the maximum depth of substitution. Since  $k_2$  and  $k_3$  can be calculated in parallel, this number is three in the calculation of  $k_4$ .

Finally we report that in actual calculation (simulating parallel computation serially and comparing with RK methods on the simple basis of total number of time steps) the second and third order algorithms given above perform very well indeed. By requiring many independent parallel function evaluations for a single time step these algorithms are especially good at giving stable, qualitatively correct answers with a small number of steps which can be insufficient for a Runge-Kutta method of the same order to give meaningful results.

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